



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:11 PM BST

PDB ID : 6QIG
Title : Metalloproteinase
Authors : Kim, H.J.; Emsley, J.
Deposited on : 2019-01-18
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

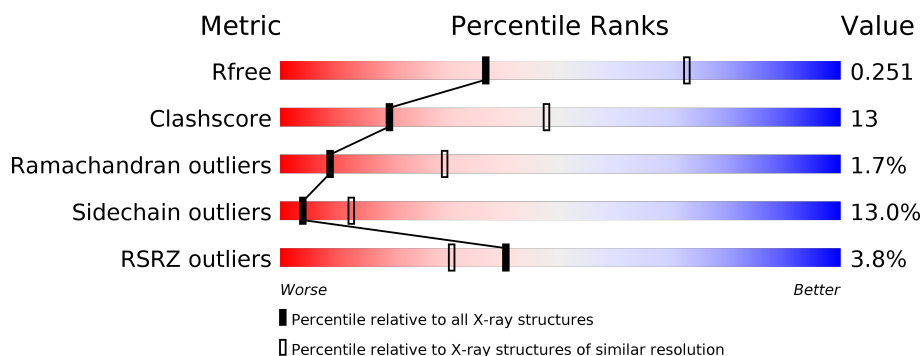
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



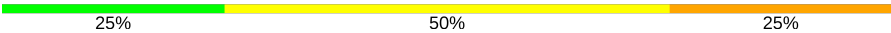
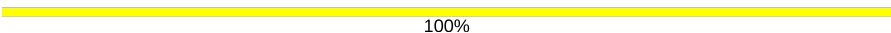
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	213	
2	H	227	
3	A	604	
4	B	3	
5	C	2	
5	F	2	

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Mol	Chain	Length	Quality of chain
6	D	4	 <div>25% 50% 25%</div>
7	E	2	 <div>100%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	PEG	A	723	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 8264 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1652	1028	278	340	6			

- Molecule 2 is a protein called Antibody Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	227	Total	C	N	O	S	0	0	0
			1715	1080	282	343	10			

- Molecule 3 is a protein called A disintegrin and metalloproteinase with thrombospondin motifs 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	581	Total	C	N	O	S	0	0	0
			4429	2735	818	837	39			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	GLN	GLU	engineered mutation	UNP Q76LX8

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



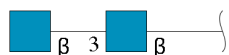
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

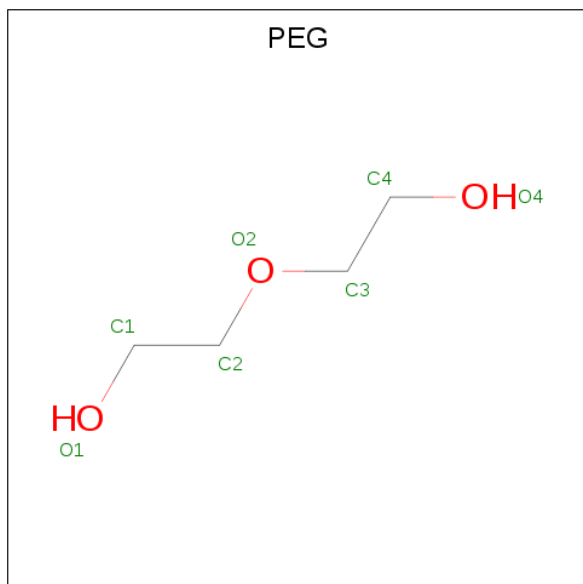
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	2	Total	Cl	0	0
			2	2		
8	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	2	Total	Cl	0	0
			2	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



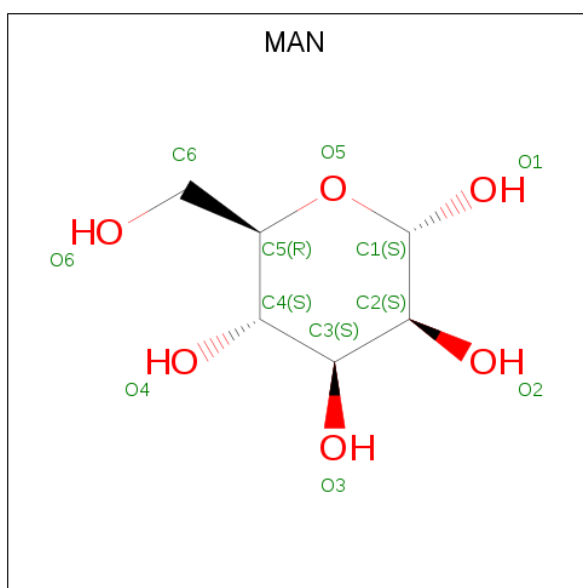
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			7	4	3		
9	L	1	Total	C	O	0	0
			7	4	3		
9	H	1	Total	C	O	0	0
			7	4	3		
9	H	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



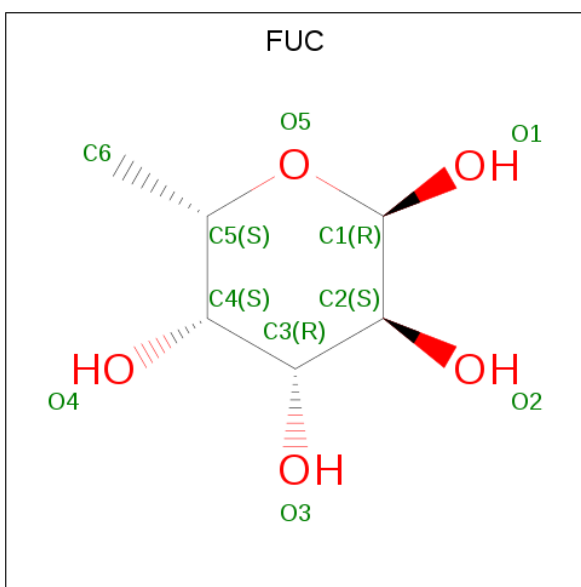
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



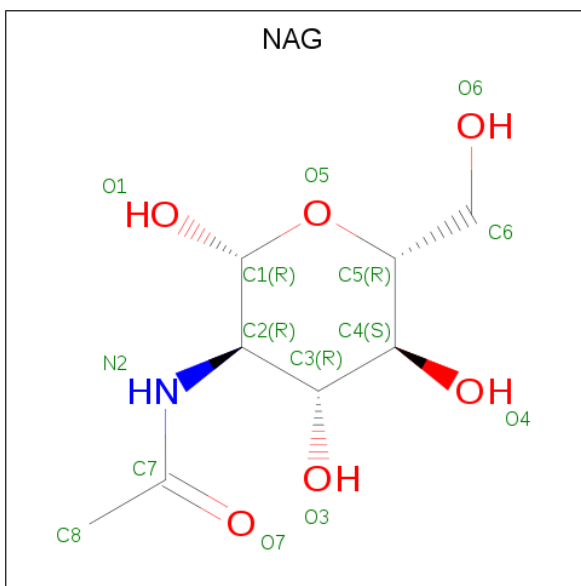
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total	C	O	0	0
			11	6	5		

- Molecule 12 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Zn 1	0	0

- Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	3	Total 3	Ca 3	0	0

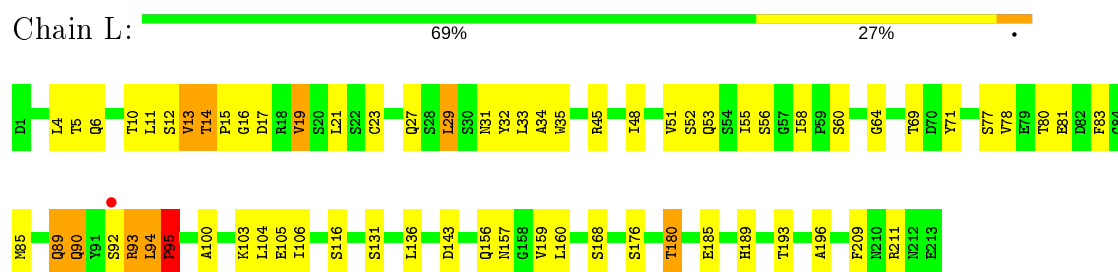
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	46	Total 46	O 46	0	0
16	H	55	Total 55	O 55	0	0
16	A	82	Total 82	O 82	0	0

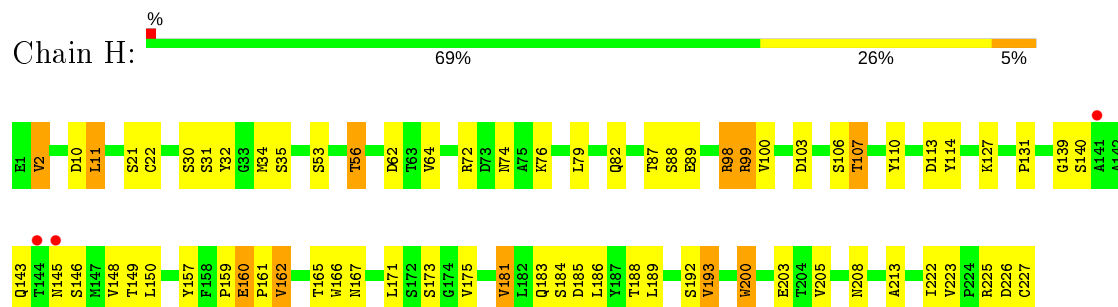
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

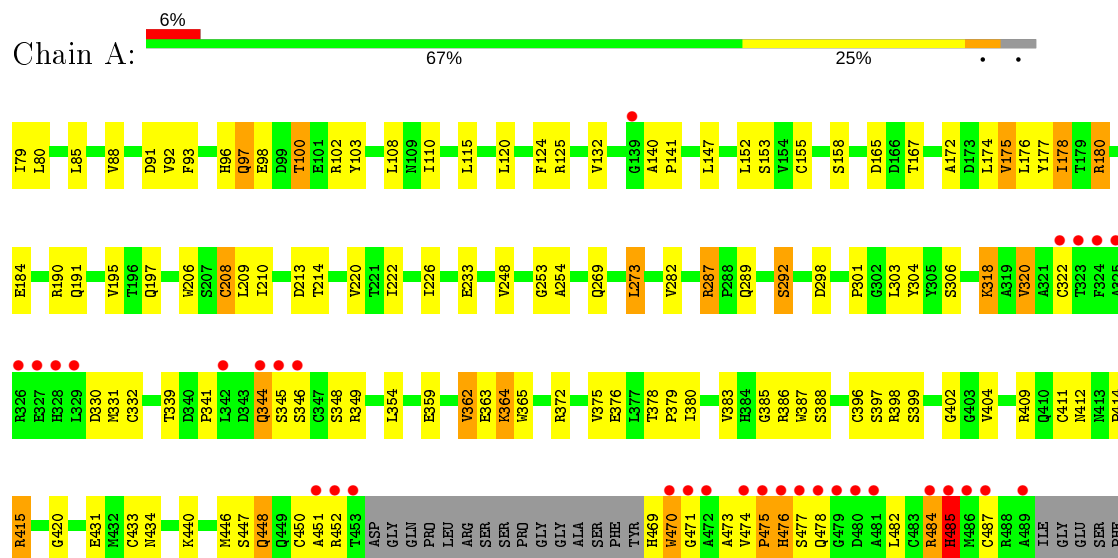
• Molecule 1: Antibody Light Chain

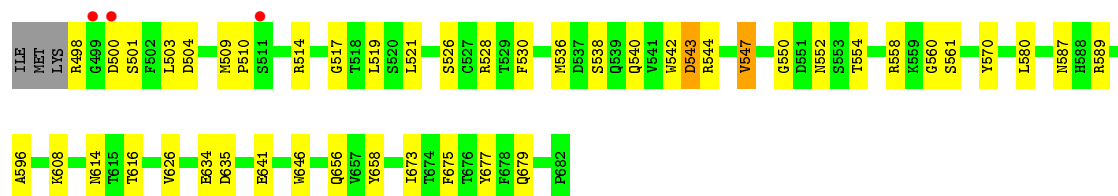


• Molecule 2: Antibody Heavy Chain



• Molecule 3: A disintegrin and metalloproteinase with thrombospondin motifs 13





- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 67% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



- Molecule 6: alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 25% 50% 25%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.53Å 87.53Å 407.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.20 – 2.80 46.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.20-2.80) 99.2 (46.16-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.205 , 0.247 0.212 , 0.251	Depositor DCC
R_{free} test set	2277 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8264	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, BMA, NAG, CL, CA, FUC, PEG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.78	0/1688	1.03	0/2291
2	H	0.72	0/1760	0.99	0/2406
3	A	0.71	0/4532	0.93	0/6160
All	All	0.73	0/7980	0.96	0/10857

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1652	0	1579	56	0
2	H	1715	0	1654	40	0
3	A	4429	0	4251	107	0
4	B	39	0	33	2	0
5	C	28	0	25	1	0
5	F	28	0	25	0	0
6	D	50	0	43	1	0
7	E	28	0	25	0	0
8	A	1	0	0	1	0
8	H	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	2	0	0	0	0
9	A	28	0	40	0	0
9	H	14	0	20	0	0
9	L	14	0	20	0	0
10	A	6	0	8	0	0
10	L	6	0	8	3	0
11	H	11	0	10	2	0
12	A	10	0	10	0	0
13	A	14	0	13	1	0
14	A	1	0	0	0	0
15	A	3	0	0	0	0
16	A	82	0	0	1	0
16	H	55	0	0	5	0
16	L	46	0	0	1	0
All	All	8264	0	7764	203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:474:VAL:CG1	3:A:475:PRO:HD3	1.56	1.33
3:A:155:CYS:SG	3:A:208:CYS:SG	1.47	1.17
3:A:474:VAL:HG12	3:A:475:PRO:HD3	1.23	1.10
3:A:396:CYS:SG	3:A:433:CYS:CB	2.39	1.08
1:L:93:ARG:O	1:L:94:LEU:HD22	1.53	1.08
3:A:474:VAL:HG13	3:A:475:PRO:HD3	1.32	1.06
1:L:93:ARG:HB3	10:L:304:GOL:O1	1.53	1.06
3:A:474:VAL:HG13	3:A:475:PRO:CD	1.89	1.03
3:A:474:VAL:CG1	3:A:475:PRO:CD	2.36	1.02
3:A:396:CYS:CB	3:A:433:CYS:SG	2.49	1.00
3:A:155:CYS:CB	3:A:208:CYS:SG	2.52	0.97
11:H:301:MAN:O5	4:B:3:BMA:H3	1.72	0.89
1:L:93:ARG:CB	10:L:304:GOL:O1	2.23	0.86
1:L:33:LEU:HD12	1:L:89:GLN:O	1.76	0.86
3:A:451:ALA:HA	3:A:469:HIS:HB2	1.64	0.79
3:A:474:VAL:HG12	3:A:475:PRO:CD	2.07	0.78
3:A:412:ASN:HA	3:A:415:ARG:HG3	1.67	0.77
2:H:87:THR:HG22	2:H:89:GLU:H	1.50	0.76
3:A:474:VAL:HG13	3:A:475:PRO:N	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:29:LEU:HD11	1:L:71:TYR:CE2	2.21	0.76
3:A:396:CYS:SG	3:A:433:CYS:SG	0.75	0.74
3:A:484:ARG:O	3:A:501:SER:HA	1.88	0.73
1:L:189:HIS:O	1:L:211:ARG:NH1	2.22	0.72
1:L:93:ARG:HG3	1:L:93:ARG:O	1.89	0.72
3:A:88:VAL:HG23	3:A:92:VAL:HG13	1.73	0.70
1:L:90:GLN:NE2	1:L:92:SER:H	1.89	0.70
3:A:473:ALA:O	3:A:477:SER:HB2	1.92	0.69
3:A:222:ILE:O	3:A:226:ILE:HG12	1.93	0.69
2:H:106:SER:OG	2:H:107:THR:N	2.27	0.68
2:H:98:ARG:NH1	2:H:113:ASP:OD1	2.28	0.67
3:A:80:LEU:HD22	3:A:282:VAL:HG23	1.76	0.67
3:A:517:GLY:HA2	3:A:542:TRP:HD1	1.59	0.66
3:A:570:TYR:CE1	3:A:658:TYR:HB2	2.31	0.66
2:H:82:GLN:HG2	16:H:430:HOH:O	1.95	0.65
1:L:14:THR:HG22	1:L:15:PRO:HD2	1.79	0.64
3:A:385:GLY:O	3:A:386:ARG:HD3	1.98	0.64
3:A:484:ARG:NH1	3:A:500:ASP:O	2.31	0.64
3:A:158:SER:HB2	3:A:175:VAL:HG11	1.80	0.63
13:A:711:NAG:H62	16:A:845:HOH:O	1.98	0.63
1:L:83:PHE:CZ	1:L:168:SER:HA	2.33	0.63
3:A:473:ALA:HB2	3:A:487:CYS:HA	1.78	0.63
2:H:100:VAL:HG22	2:H:103:ASP:OD2	1.98	0.63
3:A:141:PRO:HG2	3:A:177:TYR:CE2	2.33	0.63
1:L:92:SER:OG	1:L:92:SER:O	2.11	0.61
3:A:474:VAL:O	3:A:476:HIS:N	2.34	0.61
3:A:176:LEU:HD13	3:A:209:LEU:HD23	1.83	0.61
3:A:484:ARG:O	3:A:485:HIS:HB2	2.00	0.60
2:H:167:ASN:HD22	2:H:171:LEU:HD13	1.66	0.60
2:H:98:ARG:HH11	2:H:98:ARG:CG	2.15	0.59
3:A:306:SER:HB3	3:A:415:ARG:HH22	1.67	0.59
3:A:269:GLN:O	3:A:273:LEU:HD13	2.02	0.59
2:H:56:THR:HG23	3:A:233:GLU:OE1	2.02	0.59
3:A:155:CYS:CA	3:A:208:CYS:SG	2.92	0.58
3:A:485:HIS:HB3	3:A:498:ARG:N	2.19	0.58
2:H:200:TRP:CZ3	2:H:222:ILE:O	2.56	0.58
1:L:136:LEU:N	1:L:136:LEU:HD12	2.19	0.58
1:L:29:LEU:HD11	1:L:71:TYR:CZ	2.38	0.58
3:A:398:ARG:O	3:A:434:ASN:ND2	2.36	0.57
3:A:473:ALA:O	3:A:477:SER:CB	2.52	0.57
3:A:93:PHE:O	3:A:96:HIS:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:175:VAL:HG22	2:H:193:VAL:HG13	1.87	0.57
3:A:91:ASP:OD2	3:A:180:ARG:N	2.30	0.57
2:H:226:ASP:N	16:H:401:HOH:O	2.38	0.56
1:L:52:SER:HB3	1:L:64:GLY:O	2.05	0.56
1:L:31:ASN:O	1:L:51:VAL:HG23	2.04	0.56
3:A:253:GLY:O	3:A:254:ALA:HB3	2.04	0.56
1:L:32:TYR:HB2	1:L:92:SER:HB2	1.88	0.56
1:L:85:MET:SD	1:L:103:LYS:HG3	2.46	0.56
3:A:178:ILE:HD11	3:A:213:ASP:HB2	1.87	0.56
3:A:470:TRP:CD1	3:A:470:TRP:N	2.73	0.56
3:A:214:THR:O	8:A:720:CL:CL	2.62	0.55
3:A:528:ARG:NH1	3:A:536:MET:SD	2.80	0.55
2:H:160:GLU:O	2:H:161:PRO:C	2.43	0.55
3:A:560:GLY:HA3	3:A:675:PHE:CZ	2.42	0.55
3:A:362:VAL:HG13	3:A:364:LYS:HD2	1.88	0.54
3:A:510:PRO:HG2	3:A:514:ARG:HB3	1.88	0.54
1:L:90:GLN:HE21	1:L:92:SER:H	1.56	0.54
3:A:519:LEU:HD12	3:A:519:LEU:N	2.22	0.54
3:A:102:ARG:CZ	3:A:304:TYR:CE2	2.91	0.53
3:A:517:GLY:CA	3:A:542:TRP:HD1	2.22	0.53
3:A:155:CYS:HA	3:A:208:CYS:SG	2.48	0.53
3:A:167:THR:O	3:A:287:ARG:HD3	2.08	0.53
2:H:99:ARG:HD3	2:H:110:TYR:O	2.09	0.53
3:A:147:LEU:HD21	3:A:195:VAL:HG21	1.91	0.53
2:H:98:ARG:NH1	2:H:113:ASP:CG	2.63	0.52
1:L:131:SER:OG	1:L:180:THR:HB	2.09	0.52
3:A:176:LEU:HD13	3:A:209:LEU:CD2	2.39	0.52
2:H:166:TRP:CE2	2:H:193:VAL:HG22	2.45	0.52
1:L:29:LEU:C	1:L:29:LEU:HD12	2.30	0.52
2:H:200:TRP:HZ3	2:H:222:ILE:O	1.93	0.52
3:A:102:ARG:HD2	3:A:304:TYR:CD2	2.44	0.52
3:A:402:GLY:N	3:A:434:ASN:O	2.42	0.51
2:H:98:ARG:NH1	2:H:113:ASP:OD2	2.40	0.51
1:L:83:PHE:HZ	1:L:168:SER:HA	1.75	0.51
2:H:2:VAL:HG21	2:H:114:TYR:CG	2.46	0.51
2:H:72:ARG:CD	2:H:74:ASN:OD1	2.58	0.51
1:L:85:MET:SD	1:L:103:LYS:HA	2.51	0.51
2:H:225:ARG:N	16:H:401:HOH:O	2.42	0.51
3:A:543:ASP:HB2	3:A:547:VAL:O	2.10	0.51
2:H:62:ASP:OD1	8:H:303:CL:CL	2.66	0.51
1:L:83:PHE:HB2	1:L:104:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:LEU:HD21	1:L:196:ALA:HB2	1.94	0.50
3:A:332:CYS:HA	3:A:354:LEU:HD12	1.94	0.50
1:L:27:GLN:C	1:L:69:THR:CG2	2.80	0.50
2:H:189:LEU:C	2:H:189:LEU:HD12	2.32	0.49
3:A:80:LEU:HD22	3:A:282:VAL:CG2	2.41	0.49
1:L:13:VAL:HB	1:L:17:ASP:HB3	1.94	0.49
1:L:4:LEU:HD11	1:L:29:LEU:HD23	1.94	0.49
3:A:587:ASN:HB3	3:A:641:GLU:HB2	1.95	0.49
1:L:21:LEU:HD22	1:L:35:TRP:CZ3	2.47	0.49
3:A:447:SER:O	3:A:450:CYS:N	2.46	0.49
1:L:34:ALA:HA	1:L:48:ILE:O	2.13	0.49
3:A:120:LEU:O	3:A:120:LEU:HG	2.13	0.48
3:A:115:LEU:HB3	3:A:124:PHE:HB2	1.93	0.48
1:L:12:SER:O	1:L:13:VAL:HG13	2.13	0.48
2:H:227:CYS:HA	16:H:407:HOH:O	2.13	0.48
3:A:544:ARG:HG2	3:A:552:ASN:OD1	2.14	0.48
3:A:440:LYS:HD3	3:A:448:GLN:HE22	1.79	0.48
3:A:292:SER:O	3:A:292:SER:OG	2.30	0.48
2:H:98:ARG:HH11	2:H:98:ARG:HG3	1.79	0.47
3:A:85:LEU:C	3:A:85:LEU:HD23	2.35	0.47
3:A:378:THR:HA	3:A:380:ILE:N	2.29	0.47
1:L:27:GLN:C	1:L:69:THR:HG22	2.35	0.47
2:H:150:LEU:HD12	2:H:205:VAL:HG11	1.96	0.47
2:H:159:PRO:HD2	2:H:213:ALA:HB3	1.97	0.47
3:A:614:ASN:ND2	6:D:1:NAG:H83	2.29	0.46
2:H:72:ARG:HD3	2:H:74:ASN:OD1	2.15	0.46
3:A:320:VAL:HG12	3:A:320:VAL:O	2.15	0.46
2:H:72:ARG:HD2	2:H:74:ASN:OD1	2.15	0.46
2:H:160:GLU:O	2:H:162:VAL:N	2.49	0.46
2:H:32:TYR:O	2:H:72:ARG:NH2	2.39	0.46
1:L:11:LEU:HD13	1:L:19:VAL:HG22	1.98	0.46
1:L:14:THR:O	1:L:17:ASP:HB2	2.14	0.46
3:A:85:LEU:HB2	3:A:172:ALA:HB2	1.97	0.46
3:A:375:VAL:O	3:A:378:THR:OG1	2.32	0.46
2:H:143:GLN:HB3	16:H:429:HOH:O	2.16	0.46
1:L:33:LEU:HD23	1:L:71:TYR:CB	2.46	0.46
11:H:301:MAN:O5	4:B:3:BMA:C3	2.53	0.46
3:A:560:GLY:HA3	3:A:675:PHE:CE2	2.50	0.46
1:L:209:PHE:CD2	1:L:209:PHE:C	2.89	0.45
3:A:530:PHE:N	3:A:530:PHE:CD1	2.84	0.45
3:A:547:VAL:HG12	3:A:550:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:LEU:HD13	2:H:181:VAL:CG2	2.46	0.45
3:A:108:LEU:HD23	3:A:108:LEU:HA	1.82	0.45
3:A:303:LEU:HD13	3:A:383:VAL:HG11	1.99	0.45
2:H:159:PRO:HD2	2:H:213:ALA:CB	2.46	0.45
3:A:96:HIS:O	3:A:100:THR:HG22	2.16	0.45
1:L:136:LEU:CD2	1:L:196:ALA:HB2	2.47	0.45
1:L:51:VAL:HG22	1:L:71:TYR:CD1	2.51	0.45
1:L:6:GLN:HB2	1:L:23:CYS:SG	2.56	0.45
3:A:446:MET:CE	3:A:482:LEU:HD11	2.48	0.44
3:A:372:ARG:HD3	3:A:376:GLU:OE2	2.16	0.44
3:A:387:TRP:CE3	3:A:409:ARG:HG3	2.51	0.44
1:L:94:LEU:O	1:L:95:PRO:O	2.35	0.44
3:A:85:LEU:HB2	3:A:172:ALA:CB	2.47	0.44
3:A:91:ASP:HB2	3:A:180:ARG:HB2	2.00	0.44
3:A:322:CYS:SG	3:A:322:CYS:O	2.76	0.44
3:A:387:TRP:HB3	3:A:409:ARG:HD2	2.00	0.44
5:C:2:NAG:O7	5:C:2:NAG:H3	2.17	0.44
1:L:14:THR:HG22	1:L:15:PRO:CD	2.46	0.44
1:L:83:PHE:CD1	1:L:83:PHE:O	2.70	0.44
1:L:100:ALA:HB1	16:L:431:HOH:O	2.16	0.43
1:L:45:ARG:HH12	1:L:58:ILE:HD11	1.83	0.43
3:A:97:GLN:O	3:A:100:THR:CG2	2.66	0.43
2:H:149:THR:C	2:H:150:LEU:HD23	2.39	0.43
3:A:596:ALA:HB3	3:A:656:GLN:HB2	1.99	0.43
3:A:304:TYR:CE1	3:A:414:PRO:HB3	2.53	0.43
1:L:93:ARG:HB2	10:L:304:GOL:O1	2.14	0.43
3:A:140:ALA:HB1	3:A:141:PRO:CD	2.48	0.43
3:A:378:THR:HA	3:A:379:PRO:C	2.39	0.43
3:A:616:THR:HA	3:A:626:VAL:O	2.18	0.43
2:H:10:ASP:OD1	2:H:11:LEU:N	2.50	0.43
1:L:29:LEU:CD1	1:L:29:LEU:C	2.87	0.43
3:A:248:VAL:O	3:A:254:ALA:HB2	2.18	0.43
3:A:474:VAL:O	3:A:475:PRO:C	2.57	0.43
2:H:131:PRO:HB3	2:H:157:TYR:HB3	2.01	0.43
1:L:78:VAL:HG13	1:L:106:ILE:HD11	2.01	0.43
3:A:561:SER:HA	3:A:673:ILE:O	2.19	0.42
2:H:200:TRP:CH2	2:H:222:ILE:O	2.72	0.42
3:A:103:TYR:OH	3:A:213:ASP:OD1	2.30	0.42
1:L:51:VAL:CG2	1:L:71:TYR:CE1	3.03	0.42
3:A:318:LYS:HG3	3:A:341:PRO:HG3	2.02	0.42
3:A:197:GLN:HB3	3:A:206:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:LEU:HD11	2:H:183:GLN:CG	2.50	0.42
3:A:404:VAL:HG22	3:A:504:ASP:HB3	2.01	0.42
2:H:34:MET:HB3	2:H:79:LEU:HD22	2.00	0.42
3:A:176:LEU:HG	3:A:176:LEU:O	2.19	0.42
3:A:364:LYS:HA	3:A:365:TRP:CE3	2.55	0.42
3:A:397:SER:HB2	3:A:504:ASP:O	2.21	0.41
3:A:580:LEU:HD22	3:A:677:TYR:CE2	2.55	0.41
3:A:141:PRO:CG	3:A:177:TYR:CE2	3.02	0.41
3:A:558:ARG:HG3	3:A:679:GLN:OE1	2.20	0.41
3:A:544:ARG:CG	3:A:552:ASN:OD1	2.68	0.41
1:L:160:LEU:HD13	2:H:181:VAL:HG22	2.01	0.41
1:L:16:GLY:HA2	1:L:77:SER:HA	2.02	0.41
3:A:110:ILE:CD1	3:A:301:PRO:HG2	2.50	0.41
3:A:344:GLN:C	3:A:346:SER:H	2.24	0.41
1:L:33:LEU:HA	1:L:33:LEU:HD12	1.89	0.41
1:L:106:ILE:HA	1:L:106:ILE:HD13	1.95	0.40
1:L:29:LEU:O	1:L:92:SER:HB2	2.21	0.40
1:L:94:LEU:HD13	1:L:94:LEU:HA	1.46	0.40
1:L:51:VAL:HG21	1:L:71:TYR:CE1	2.56	0.40
3:A:184:GLU:OE1	3:A:190:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	211/213 (99%)	200 (95%)	9 (4%)	2 (1%)	17	46
2	H	225/227 (99%)	204 (91%)	17 (8%)	4 (2%)	8	28
3	A	575/604 (95%)	496 (86%)	68 (12%)	11 (2%)	8	26
All	All	1011/1044 (97%)	900 (89%)	94 (9%)	17 (2%)	9	29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	95	PRO
3	A	345	SER
3	A	448	GLN
3	A	485	HIS
2	H	140	SER
3	A	348	SER
3	A	543	ASP
2	H	184	SER
3	A	388	SER
3	A	475	PRO
1	L	60	SER
3	A	132	VAL
3	A	362	VAL
2	H	99	ARG
3	A	420	GLY
2	H	139	GLY
3	A	471	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	189/189 (100%)	163 (86%)	26 (14%)	3	11
2	H	194/194 (100%)	162 (84%)	32 (16%)	2	7
3	A	480/498 (96%)	426 (89%)	54 (11%)	6	18
All	All	863/881 (98%)	751 (87%)	112 (13%)	4	13

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	10	THR
1	L	13	VAL
1	L	14	THR

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Mol	Chain	Res	Type
1	L	19	VAL
1	L	29	LEU
1	L	53	GLN
1	L	55	ILE
1	L	56	SER
1	L	80	THR
1	L	81	GLU
1	L	89	GLN
1	L	90	GLN
1	L	93	ARG
1	L	94	LEU
1	L	95	PRO
1	L	105	GLU
1	L	116	SER
1	L	143	ASP
1	L	156	GLN
1	L	157	ASN
1	L	159	VAL
1	L	176	SER
1	L	180	THR
1	L	185	GLU
1	L	193	THR
2	H	2	VAL
2	H	11	LEU
2	H	21	SER
2	H	22	CYS
2	H	30	SER
2	H	31	SER
2	H	35	SER
2	H	53	SER
2	H	56	THR
2	H	64	VAL
2	H	76	LYS
2	H	88	SER
2	H	98	ARG
2	H	107	THR
2	H	127	LYS
2	H	145	ASN
2	H	146	SER
2	H	148	VAL
2	H	160	GLU
2	H	162	VAL

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Mol	Chain	Res	Type
2	H	165	THR
2	H	173	SER
2	H	181	VAL
2	H	185	ASP
2	H	186	LEU
2	H	188	THR
2	H	192	SER
2	H	193	VAL
2	H	200	TRP
2	H	203	GLU
2	H	208	ASN
2	H	223	VAL
3	A	79	ILE
3	A	97	GLN
3	A	98	GLU
3	A	100	THR
3	A	125	ARG
3	A	152	LEU
3	A	153	SER
3	A	165	ASP
3	A	174	LEU
3	A	175	VAL
3	A	178	ILE
3	A	180	ARG
3	A	191	GLN
3	A	208	CYS
3	A	210	ILE
3	A	220	VAL
3	A	273	LEU
3	A	287	ARG
3	A	289	GLN
3	A	292	SER
3	A	298	ASP
3	A	318	LYS
3	A	320	VAL
3	A	330	ASP
3	A	331	MET
3	A	339	THR
3	A	344	GLN
3	A	349	ARG
3	A	359	GLU
3	A	363	GLU

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Mol	Chain	Res	Type
3	A	364	LYS
3	A	399	SER
3	A	411	CYS
3	A	415	ARG
3	A	431	GLU
3	A	452	ARG
3	A	470	TRP
3	A	476	HIS
3	A	478	GLN
3	A	484	ARG
3	A	485	HIS
3	A	503	LEU
3	A	509	MET
3	A	521	LEU
3	A	526	SER
3	A	538	SER
3	A	540	GLN
3	A	547	VAL
3	A	554	THR
3	A	589	ARG
3	A	608	LYS
3	A	634	GLU
3	A	635	ASP
3	A	646	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	90	GLN
2	H	3	GLN
2	H	143	GLN
2	H	167	ASN
3	A	97	GLN
3	A	123	GLN
3	A	191	GLN
3	A	448	GLN
3	A	485	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

13 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	B	1	3,4	14,14,15	0.91	1 (7%)	17,19,21	1.10	1 (5%)
4	NAG	B	2	4	14,14,15	1.39	1 (7%)	17,19,21	1.79	4 (23%)
4	BMA	B	3	4	11,11,12	0.57	0	15,15,17	1.68	4 (26%)
5	NAG	C	1	5	14,14,15	0.74	0	17,19,21	1.85	3 (17%)
5	NAG	C	2	5	14,14,15	0.28	0	17,19,21	0.65	0
6	NAG	D	1	3,6	14,14,15	0.65	0	17,19,21	2.11	6 (35%)
6	NAG	D	2	6	14,14,15	0.69	0	17,19,21	1.51	3 (17%)
6	BMA	D	3	6	11,11,12	0.41	0	15,15,17	1.02	0
6	MAN	D	4	6	11,11,12	0.96	1 (9%)	15,15,17	2.07	3 (20%)
7	NAG	E	1	3,7	14,14,15	0.82	0	17,19,21	2.25	5 (29%)
7	NAG	E	2	7	14,14,15	0.64	0	17,19,21	1.64	4 (23%)
5	NAG	F	1	3,5	14,14,15	0.98	0	17,19,21	1.68	1 (5%)
5	NAG	F	2	5	14,14,15	0.94	1 (7%)	17,19,21	2.64	6 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	0/1/1/1
5	NAG	C	1	5	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	4/6/23/26	0/1/1/1
6	NAG	D	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	BMA	D	3	6	-	1/2/19/22	0/1/1/1
6	MAN	D	4	6	-	2/2/19/22	0/1/1/1
7	NAG	E	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1
5	NAG	F	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	5/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2	NAG	C1-C2	2.60	1.56	1.52
4	B	2	NAG	O5-C1	-2.58	1.39	1.43
6	D	4	MAN	C2-C3	2.38	1.56	1.52
4	B	1	NAG	C2-N2	-2.05	1.42	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	4	MAN	C1-C2-C3	5.94	116.97	109.67
7	E	1	NAG	O5-C1-C2	-5.48	102.63	111.29
5	F	2	NAG	C1-O5-C5	5.36	119.46	112.19
5	F	2	NAG	C2-N2-C7	5.18	130.28	122.90
4	B	2	NAG	O4-C4-C3	-5.11	98.54	110.35
5	F	1	NAG	O5-C1-C2	-4.62	103.99	111.29
5	C	1	NAG	C3-C4-C5	4.11	117.57	110.24
5	F	2	NAG	C4-C3-C2	4.11	117.04	111.02
5	C	1	NAG	O5-C5-C6	-4.02	100.91	107.20
5	F	2	NAG	C8-C7-N2	3.99	122.86	116.10
7	E	1	NAG	O3-C3-C4	3.98	119.54	110.35
6	D	1	NAG	C2-N2-C7	3.83	128.36	122.90
6	D	1	NAG	O5-C5-C4	-3.77	101.65	110.83
6	D	1	NAG	C8-C7-N2	3.74	122.43	116.10
5	C	1	NAG	C1-O5-C5	3.68	117.18	112.19
4	B	3	BMA	O2-C2-C1	3.63	116.58	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	2	NAG	C4-C3-C2	3.58	116.27	111.02
7	E	2	NAG	C2-N2-C7	-3.40	118.06	122.90
7	E	2	NAG	C1-O5-C5	-3.39	107.60	112.19
5	F	2	NAG	O5-C5-C6	3.22	112.25	107.20
7	E	1	NAG	O4-C4-C5	-3.13	101.53	109.30
6	D	4	MAN	O5-C5-C4	-3.13	103.22	110.83
6	D	1	NAG	O7-C7-N2	-3.04	116.36	121.95
4	B	2	NAG	O5-C1-C2	-3.03	106.50	111.29
4	B	3	BMA	O2-C2-C3	-2.97	104.19	110.14
6	D	2	NAG	O7-C7-N2	-2.91	116.60	121.95
6	D	2	NAG	C8-C7-N2	2.82	120.88	116.10
6	D	2	NAG	C3-C4-C5	2.79	115.22	110.24
6	D	1	NAG	C6-C5-C4	2.65	119.20	113.00
5	F	2	NAG	O7-C7-C8	-2.62	117.19	122.06
7	E	1	NAG	O3-C3-C2	-2.48	104.33	109.47
4	B	3	BMA	C1-C2-C3	2.44	112.67	109.67
7	E	1	NAG	O5-C5-C4	-2.43	104.91	110.83
4	B	3	BMA	O5-C5-C6	2.18	110.62	107.20
6	D	4	MAN	C2-C3-C4	2.16	114.63	110.89
4	B	2	NAG	C1-O5-C5	-2.11	109.33	112.19
7	E	2	NAG	O5-C5-C4	-2.11	105.69	110.83
6	D	1	NAG	C1-O5-C5	-2.10	109.34	112.19
4	B	2	NAG	C2-N2-C7	-2.07	119.95	122.90
4	B	1	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
6	D	4	MAN	O5-C5-C6-O6
6	D	4	MAN	C4-C5-C6-O6
7	E	2	NAG	O5-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
7	E	2	NAG	C4-C5-C6-O6
5	C	2	NAG	C1-C2-N2-C7
6	D	2	NAG	C8-C7-N2-C2
6	D	2	NAG	O7-C7-N2-C2
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2

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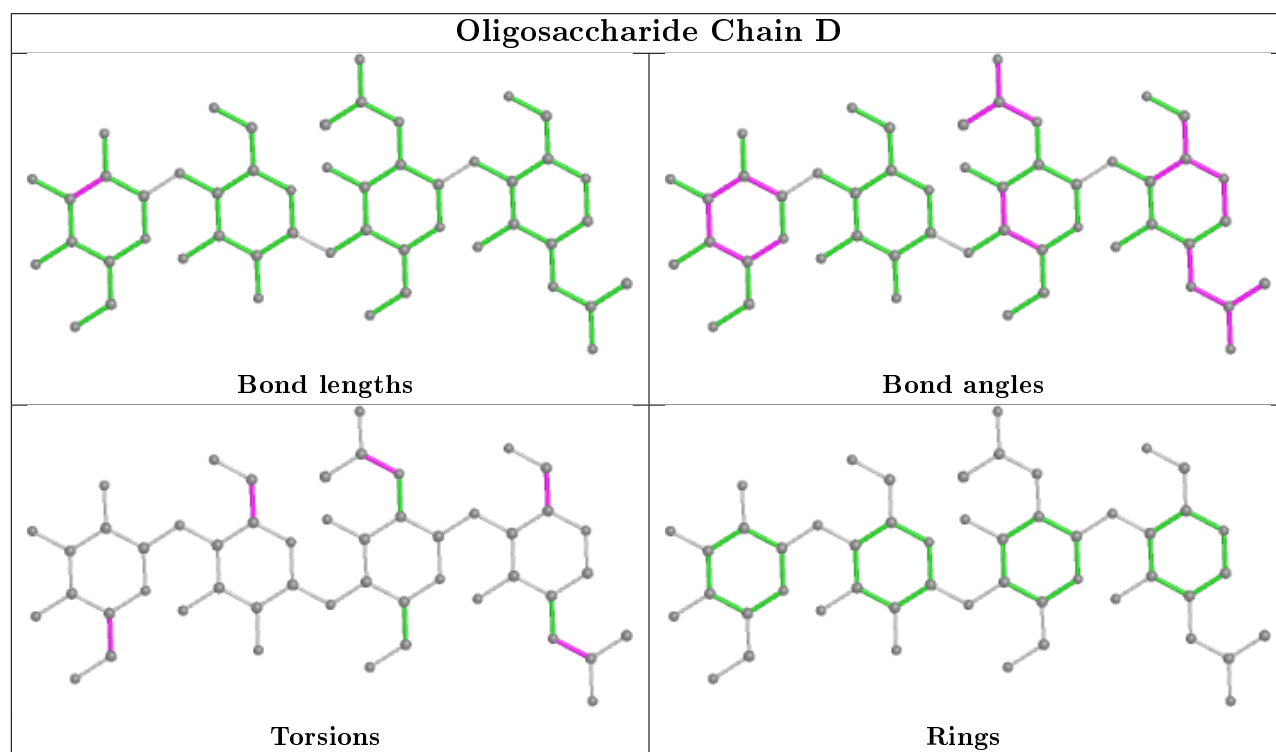
Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C8-C7-N2-C2
6	D	1	NAG	O7-C7-N2-C2
4	B	3	BMA	O5-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
6	D	3	BMA	O5-C5-C6-O6
5	C	2	NAG	C3-C2-N2-C7
6	D	1	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
4	B	3	BMA	C4-C5-C6-O6
5	F	2	NAG	C3-C2-N2-C7
4	B	2	NAG	C8-C7-N2-C2
5	F	1	NAG	C4-C5-C6-O6

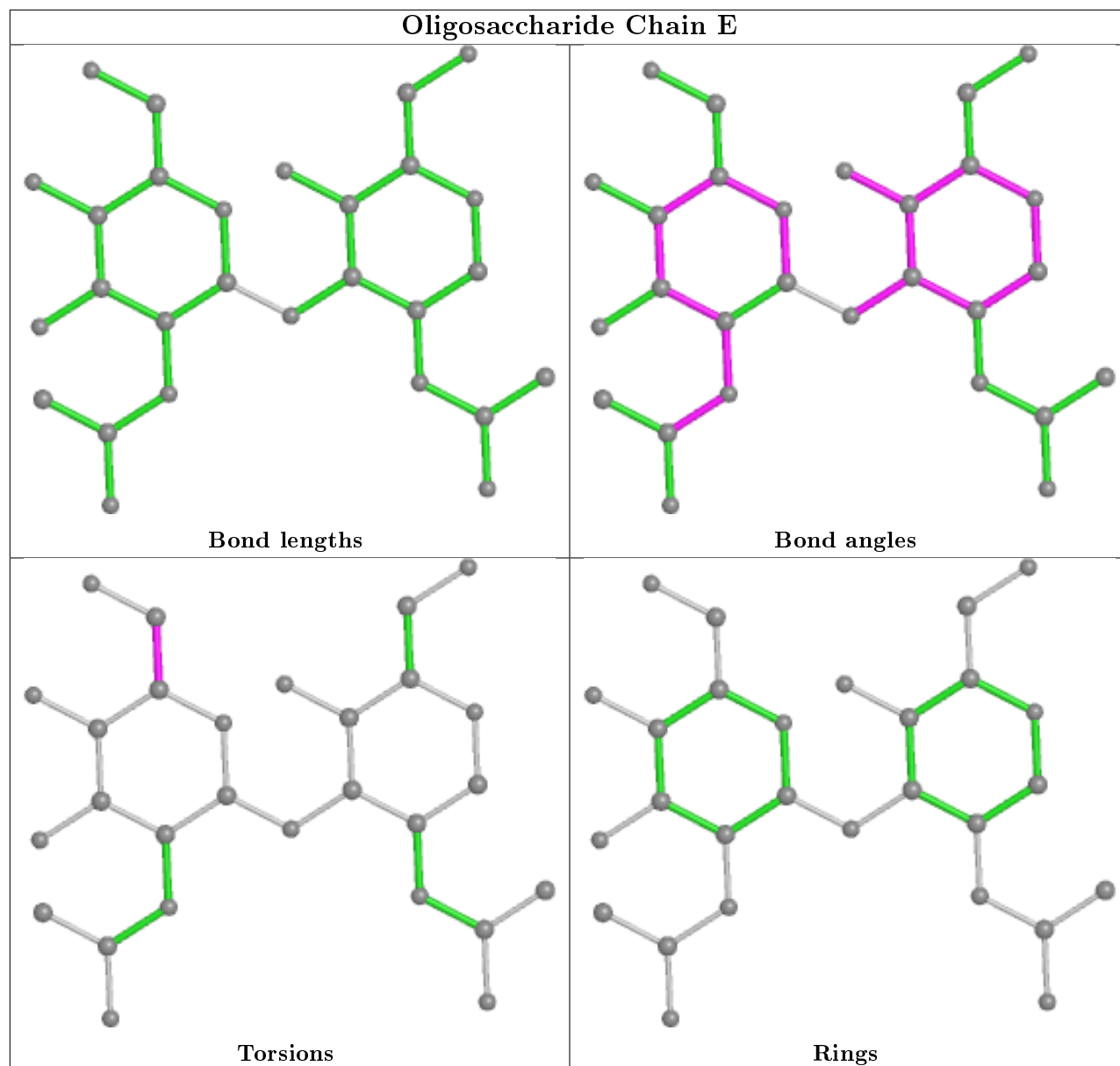
There are no ring outliers.

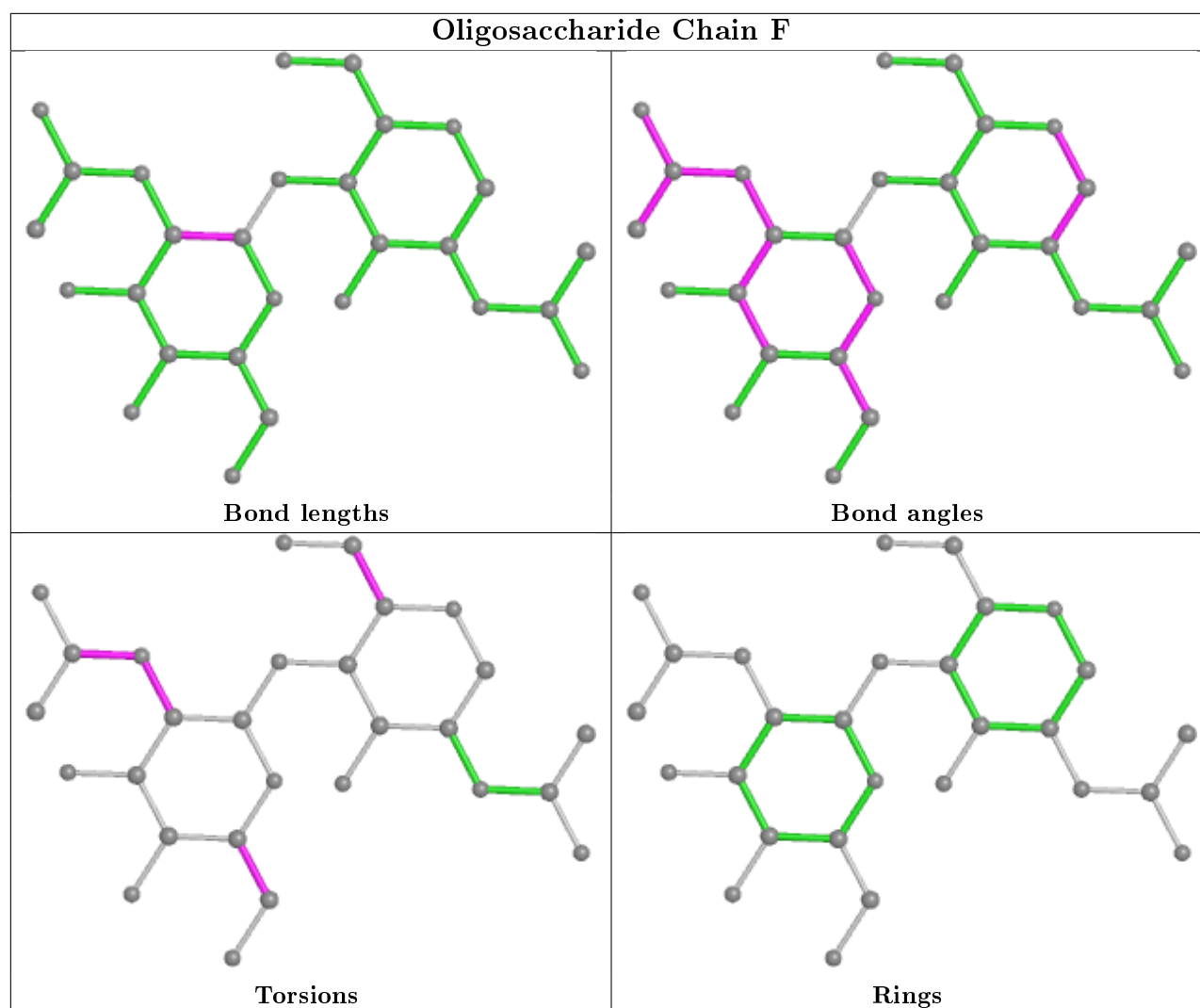
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3	BMA	2	0
6	D	1	NAG	1	0
5	C	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	MAN	H	301	-	11,11,12	0.74	0	15,15,17	2.04	4 (26%)
9	PEG	H	305	-	6,6,6	0.38	0	5,5,5	0.25	0
9	PEG	A	721	-	6,6,6	0.15	0	5,5,5	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	A	724	-	5,5,5	0.17	0	5,5,5	0.32	0
9	PEG	A	725	-	6,6,6	0.43	0	5,5,5	0.25	0
12	FUC	A	710	3	10,10,11	0.69	0	14,14,16	1.16	1 (7%)
9	PEG	A	722	-	6,6,6	0.41	0	5,5,5	0.22	0
10	GOL	L	304	-	5,5,5	0.24	0	5,5,5	0.45	0
13	NAG	A	711	3	14,14,15	0.60	0	17,19,21	2.36	5 (29%)
9	PEG	L	305	-	6,6,6	0.16	0	5,5,5	0.10	0
9	PEG	H	304	-	6,6,6	0.23	0	5,5,5	0.18	0
9	PEG	L	303	-	6,6,6	0.13	0	5,5,5	0.16	0
9	PEG	A	723	-	6,6,6	0.28	0	5,5,5	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	H	301	-	-	1/2/19/22	0/1/1/1
9	PEG	H	305	-	-	2/4/4/4	-
9	PEG	A	721	-	-	3/4/4/4	-
10	GOL	A	724	-	-	2/4/4/4	-
9	PEG	A	725	-	-	3/4/4/4	-
12	FUC	A	710	3	-	-	0/1/1/1
9	PEG	A	722	-	-	1/4/4/4	-
10	GOL	L	304	-	-	3/4/4/4	-
13	NAG	A	711	3	-	4/6/23/26	0/1/1/1
9	PEG	L	305	-	-	2/4/4/4	-
9	PEG	H	304	-	-	4/4/4/4	-
9	PEG	L	303	-	-	3/4/4/4	-
9	PEG	A	723	-	-	3/4/4/4	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	301	MAN	C1-O5-C5	4.90	118.83	112.19
13	A	711	NAG	C1-O5-C5	4.89	118.81	112.19
13	A	711	NAG	C4-C3-C2	-4.66	104.19	111.02
13	A	711	NAG	C1-C2-N2	-4.10	103.48	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	711	NAG	O5-C1-C2	3.41	116.67	111.29
11	H	301	MAN	C3-C4-C5	3.40	116.30	110.24
11	H	301	MAN	C1-C2-C3	3.27	113.69	109.67
12	A	710	FUC	O3-C3-C4	2.58	116.31	110.35
13	A	711	NAG	O5-C5-C6	2.52	111.16	107.20
11	H	301	MAN	O5-C5-C6	2.13	110.54	107.20

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	L	304	GOL	C1-C2-C3-O3
10	A	724	GOL	C1-C2-C3-O3
13	A	711	NAG	C8-C7-N2-C2
13	A	711	NAG	O7-C7-N2-C2
13	A	711	NAG	C4-C5-C6-O6
9	A	722	PEG	O1-C1-C2-O2
9	A	725	PEG	O2-C3-C4-O4
10	L	304	GOL	O1-C1-C2-C3
9	L	303	PEG	O1-C1-C2-O2
10	L	304	GOL	O2-C2-C3-O3
10	A	724	GOL	O2-C2-C3-O3
9	A	723	PEG	O1-C1-C2-O2
9	H	304	PEG	O1-C1-C2-O2
13	A	711	NAG	O5-C5-C6-O6
9	H	305	PEG	O2-C3-C4-O4
9	A	723	PEG	O2-C3-C4-O4
9	A	725	PEG	O1-C1-C2-O2
9	A	721	PEG	C4-C3-O2-C2
9	L	305	PEG	C4-C3-O2-C2
9	L	305	PEG	C1-C2-O2-C3
9	A	723	PEG	C1-C2-O2-C3
9	H	304	PEG	O2-C3-C4-O4
9	H	304	PEG	C4-C3-O2-C2
9	A	721	PEG	O1-C1-C2-O2
9	A	725	PEG	C4-C3-O2-C2
9	L	303	PEG	C4-C3-O2-C2
11	H	301	MAN	C4-C5-C6-O6
9	A	721	PEG	C1-C2-O2-C3
9	L	303	PEG	C1-C2-O2-C3
9	H	304	PEG	C1-C2-O2-C3
9	H	305	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	301	MAN	2	0
10	L	304	GOL	3	0
13	A	711	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	L	213/213 (100%)	-0.41	1 (0%)	91 88	24, 37, 63, 103	0
2	H	227/227 (100%)	-0.34	3 (1%)	77 72	26, 44, 78, 125	0
3	A	581/604 (96%)	0.03	35 (6%)	21 14	19, 61, 130, 173	0
All	All	1021/1044 (97%)	-0.15	39 (3%)	40 30	19, 52, 110, 173	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	476	HIS	7.5
3	A	478	GLN	6.7
3	A	328	HIS	6.6
3	A	324	PHE	6.1
3	A	471	GLY	6.0
3	A	329	LEU	5.6
3	A	451	ALA	5.3
3	A	323	THR	4.9
3	A	499	GLY	4.0
3	A	327	GLU	4.0
3	A	452	ARG	3.8
3	A	500	ASP	3.5
3	A	472	ALA	3.5
3	A	485	HIS	3.4
3	A	479	GLY	3.3
3	A	345	SER	3.2
3	A	489	ALA	3.1
2	H	145	ASN	3.1
3	A	475	PRO	3.0
3	A	486	MET	2.8
3	A	511	SER	2.8
1	L	92	SER	2.8
3	A	480	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	144	THR	2.7
3	A	344	GLN	2.5
3	A	477	SER	2.5
3	A	474	VAL	2.5
3	A	470	TRP	2.5
3	A	346	SER	2.4
2	H	141	ALA	2.4
3	A	487	CYS	2.3
3	A	481	ALA	2.3
3	A	326	ARG	2.2
3	A	453	THR	2.2
3	A	342	LEU	2.2
3	A	484	ARG	2.1
3	A	139	GLY	2.0
3	A	325	ALA	2.0
3	A	322	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

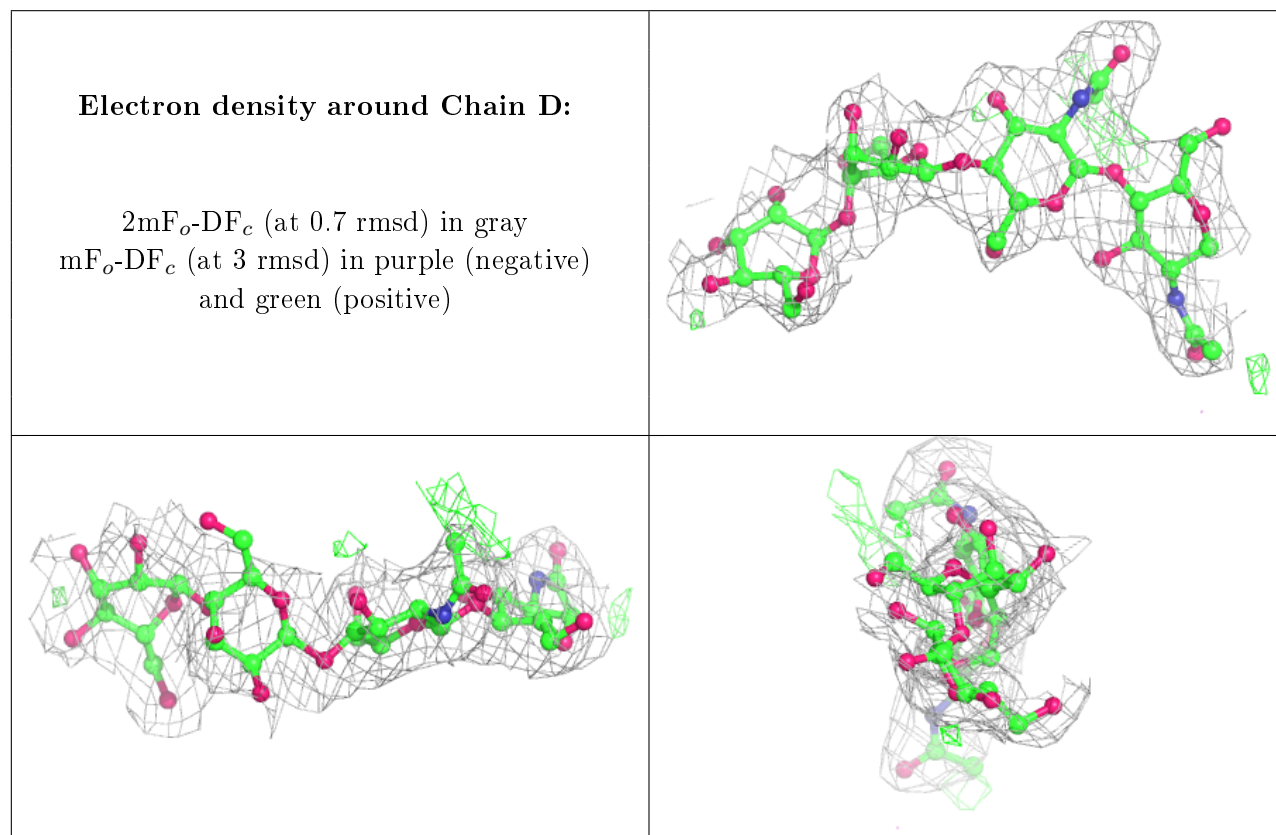
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	C	2	14/15	0.71	0.37	100,125,135,145	0
5	NAG	F	2	14/15	0.72	0.36	134,144,149,156	0
6	MAN	D	4	11/12	0.76	0.25	89,113,122,122	0
6	BMA	D	3	11/12	0.83	0.28	128,134,139,140	0
7	NAG	E	2	14/15	0.83	0.29	85,125,131,133	0
4	BMA	B	3	11/12	0.83	0.19	83,94,101,110	0
5	NAG	F	1	14/15	0.85	0.14	72,94,104,117	0
6	NAG	D	2	14/15	0.87	0.13	65,87,105,118	0
7	NAG	E	1	14/15	0.91	0.19	80,90,102,104	0
5	NAG	C	1	14/15	0.93	0.20	62,80,91,112	0
6	NAG	D	1	14/15	0.95	0.12	63,68,80,81	0
4	NAG	B	2	14/15	0.95	0.11	55,61,66,71	0

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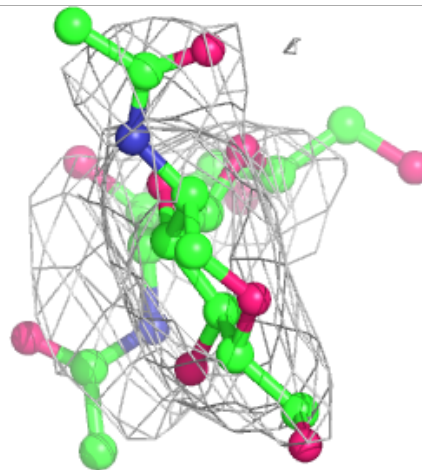
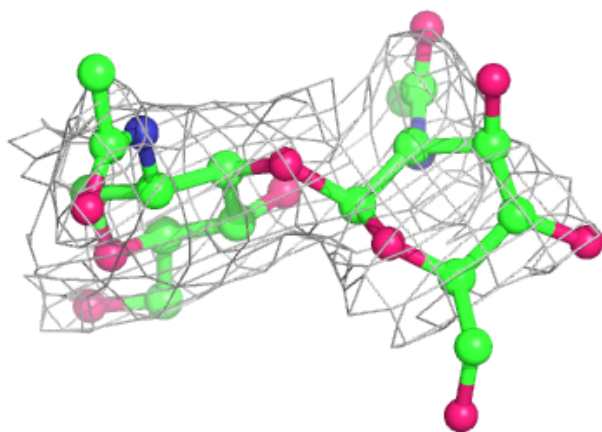
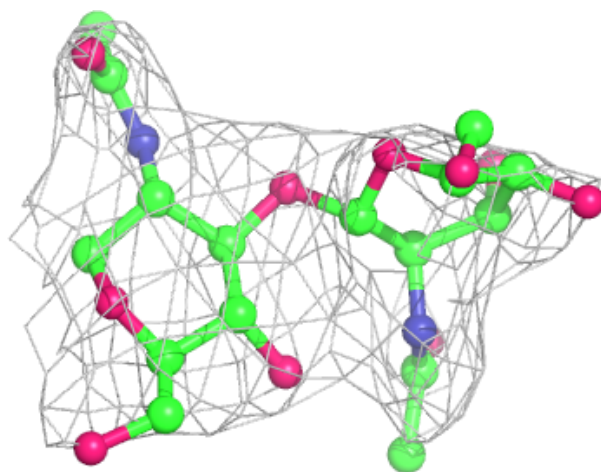
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	1	14/15	0.96	0.12	44,51,63,73	0

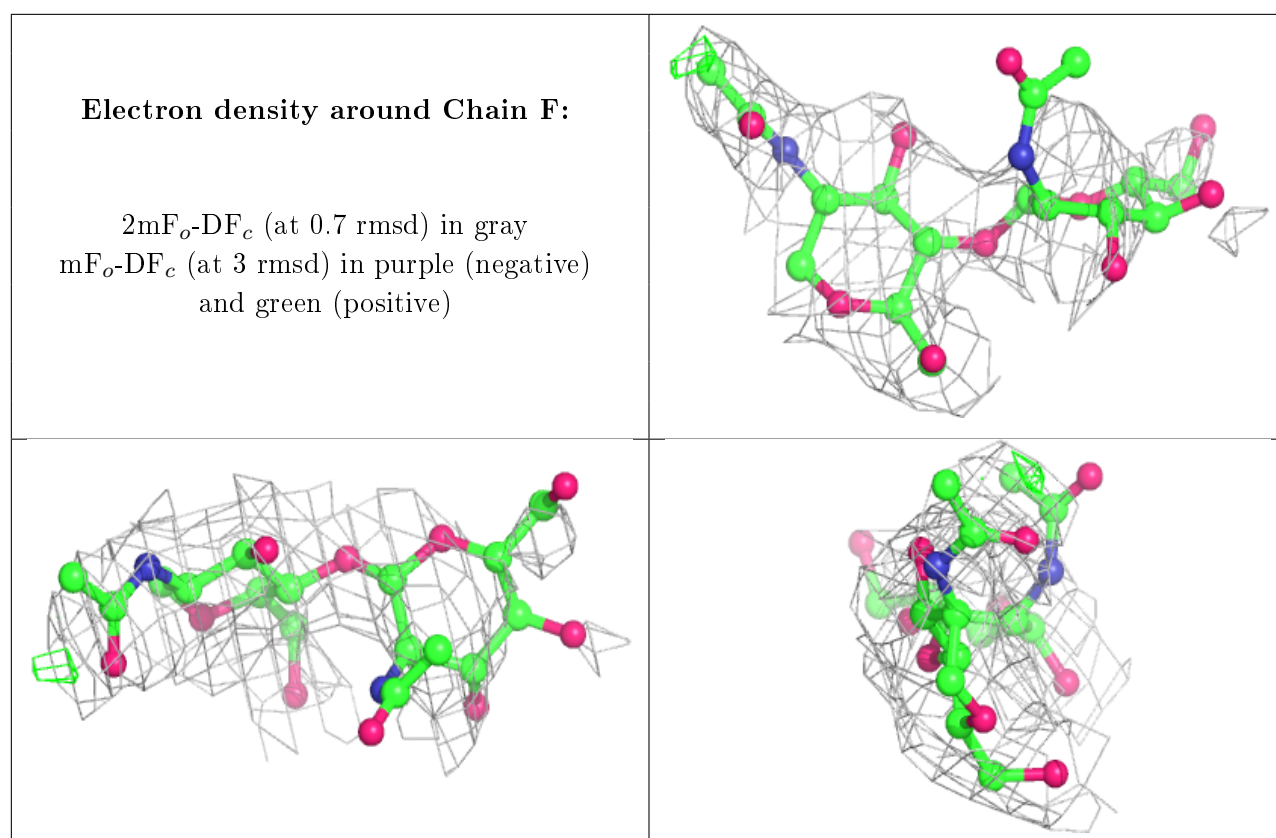
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PEG	H	304	7/7	0.62	0.35	88,97,99,107	0
9	PEG	A	723	7/7	0.65	0.46	82,100,109,110	0
9	PEG	A	722	7/7	0.71	0.30	71,73,85,87	0
9	PEG	L	305	7/7	0.74	0.18	88,96,103,103	0
8	CL	L	301	1/1	0.75	0.23	81,81,81,81	0
13	NAG	A	711	14/15	0.78	0.29	92,112,117,118	0
9	PEG	L	303	7/7	0.79	0.26	97,102,105,107	0
11	MAN	H	301	11/12	0.79	0.20	89,96,101,109	0
10	GOL	L	304	6/6	0.83	0.28	68,75,89,90	0
10	GOL	A	724	6/6	0.84	0.19	61,65,69,70	0
9	PEG	H	305	7/7	0.85	0.21	62,73,83,83	0
8	CL	A	720	1/1	0.88	0.10	65,65,65,65	0
8	CL	H	302	1/1	0.89	0.18	79,79,79,79	0
9	PEG	A	725	7/7	0.90	0.21	65,76,83,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CA	A	718	1/1	0.91	0.06	73,73,73,73	0
9	PEG	A	721	7/7	0.92	0.16	89,96,98,100	0
8	CL	H	303	1/1	0.93	0.07	86,86,86,86	0
12	FUC	A	710	10/11	0.96	0.26	45,59,63,64	0
15	CA	A	717	1/1	0.96	0.06	51,51,51,51	0
8	CL	L	302	1/1	0.96	0.14	60,60,60,60	0
15	CA	A	719	1/1	0.98	0.05	79,79,79,79	0
14	ZN	A	716	1/1	1.00	0.15	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.